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Higher-dimensional Dedekind sums and their bounds arising from the discrete diagonal of the n-cube

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Abstract

Higher-dimensional Dedekind sums are defined as a generalization of a recent one-dimensional probability model of Dilcher and Girstmair to a d-dimensional cube. The analysis of the frequency distribution of diagonal lattice points leads to new formulae in certain special cases, and also to new bounds for the classical Dedekind sums. We define a new correspondence between n-dimensional Dedekind sums and certain convex n-dimensional cones, and we conjecture that these cones have a largest spacial angle of $\pi/6$. Bounds on n-dimensional Dedekind sums are important in the enumeration of lattice points in polytopes, since they are the building blocks for the lattice point enumerator of a polytope. Here, upper bounds for n-dimensional Dedekind sums are expressed in terms of 1-dimensional moments, and various relations among the moments are derived using statistical methods.
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Counting pairs is the oldest trick in combinatorics ... Every time we count pairs, we learn something from it.

Gil Kalai

1. Introduction

Historically, Dedekind sums first appeared in Dedekind's transformation law of his η-function [2]. Dedekind sums have since become an integral part of combinatorial geometry (lattice point enumeration [8]), algebraic number theory (class number formulae [7]), topology (signature defects of manifolds [4]), and algorithmic complexity (pseudo random number generators [5]). We begin by defining the classical Dedekind sum, whose basic ingredient is the sawtooth function

$$((x)) = \begin{cases} \{x\} - \frac{1}{2}, & \text{if } x \notin \mathbb{Z}, \\ 0, & \text{if } x \in \mathbb{Z}. \end{cases}$$

Here $\{x\} = x - \lfloor x \rfloor$ denotes the fractional part of a real number x.

For any two positive integers a and b, we define the *classical Dedekind sum* as

$$s(a,b) = \sum_{k \bmod b} \left(\left(\frac{ka}{b}\right)\right)\left(\left(\frac{k}{b}\right)\right). \tag{1.1}$$

Here the sum is over a complete residue system modulo b.

The classic introduction to the arithmetic properties of the Dedekind sum is [9]. The Dedekind sums have recently been cast in a new light as essentially the second moments of an appealing probability model introduced by Dilcher and Girstmair [3]. They divide an interval of length a into b equal subintervals ("boxes") and count the number of integers in each subinterval.

We generalize their approach by considering a d-dimensional cube ($d \geqslant 2$) of side length $a \in \mathbb{N}$. Along the main diagonal of the this cube in d dimensions we mark the points with integer coordinates. The cube is now partitioned into $b_1 b_2 \cdots b_d$ boxes by dividing the jth side of the cube into b_j intervals of equal length. Each box is given the coordinates $(j_1, j_2, \ldots, j_d)$ where $j_k = 1, \ldots, b_k$ ($k = 1, \ldots, d$). Let $f_{a;b_1,\ldots,b_d}(j_1, \ldots, j_d)$ denote the number (frequency) of diagonal lattice points along the main diagonal of the cube which belong to the $(j_1, j_2, \ldots, j_d)$ box.

The generalized Dedekind sums under consideration are

$$\begin{aligned} S_d(a;\mathbf{b}) &= S_d(a; b_1, b_2, \ldots, b_d) \\ &= \frac{1}{a} \sum_{k_1=0}^{b_1-1} \cdots \sum_{k_d=0}^{b_d-1} k_1 \cdots k_d \, f_{a;b_1,\ldots,b_d}(k_1, \ldots, k_d), \end{aligned} \tag{1.2}$$

a mixed moment for the $f_{a;b_1,\dots,b_d}$ distribution. In Section 2 we present basic definition and facts. We show that

$$S_d(a;\mathbf{b}) = \frac{1}{a}\sum_{m=0}^{a-1}\left\lfloor\frac{mb_1}{a}\right\rfloor\cdots\left\lfloor\frac{mb_d}{a}\right\rfloor. \tag{1.3}$$

For the case $d=1$ we define the kth moment as

$$M_k(a;b) = \frac{1}{a}\sum_{m=0}^{a-1}\left\lfloor\frac{mb}{a}\right\rfloor^k. \tag{1.4}$$

These moments are used in Sections 5 and 6 to provide, via the Cauchy–Schwartz inequality, upper bounds for $S_d(a;\mathbf{b})$.

The second moment $M_2(a;b)$ is of special importance since it is connected with the classical Dedekind sum $s(a,b)$ according to the formula (see Section 2)

$$M_2(a;b) = \frac{(b^2+1)(a-1)(2a-1)}{6a^2} - \frac{(a-1)b}{2a} - \frac{2b}{a}s(b,a). \tag{1.5}$$

By analyzing the structure of the univariate and bivariate frequency distributions (Section 3), we derive in Section 4 new formulae for $M_2(a;b)$, in some special cases, and provide several types of lower and upper bounds. In Section 5 we analyze the ratio of $S_2(a;b_1,b_2)$ to its upper bound $(M_2(a;b_1)M_2(a;b_2))^{1/2}$. All these ratios $R_2(a;b_1,b_2)$ are empirically found to be greater or equal to $R_2(5;2,3)=\sqrt{3}/2$, leading to the following conjecture (see Section 5.1 below):

Conjecture 1. *For all $a,b,c \geqslant 3$,*

$$R_2(a;b,c) \geqslant R_2(5;2,3) = \frac{\sqrt{3}}{2}. \tag{1.6}$$

Geometrically, $S_2(a;b_1,b_2)$ is an inner product of the vectors $\mathbf{v}_{b_1} = (\lfloor b_1/a\rfloor, \lfloor 2b_1/a\rfloor, \dots, \lfloor (a-1)b_1/a\rfloor)$ and $\mathbf{v}_{b_2} = (\lfloor b_2/a\rfloor, \lfloor 2b_2/a\rfloor, \dots, \lfloor (a-1)b_2/a\rfloor)$ in $\mathbb{R}^{a-1}$, and $R_2(a;b_1,b_2)$ is the cosine of the angle between these two vectors. It appears from both empirical and theoretical evidence that all these vectors, for $a\geqslant 3$, $b_1,b_2\geqslant 2$, are within a cone with largest possible angle of $\cos^{-1}(\sqrt{3}/2)=\pi/6$. In Section 5.1 we have some general results and observations on the functions $R_2(a;b_1,b_2)$. In Section 5.2 we analyze the geometry of the vectors $\mathbf{v}_b = (\lfloor b/a\rfloor, \lfloor 2b/a\rfloor, \dots, \lfloor (a-1)b/a\rfloor)$ and prove several lemmas, which lend further credence to the validity of Conjecture 1. Finally, in Section 6 we present higher-dimensional upper bounds for $S_d(a;\mathbf{b})$ in terms of the rth moments $M_r(a;b)$, and prove that $M_r(a;b)$ is log-convex in r. It is worth noting that when $a=b$, the rth moment $M_r(a;a)$ is essentially the rth Bernoulli polynomial, and hence these moments are a geometrically motivated generalization of the Bernoulli polynomials.

2. Generalizing the Dilcher–Girstmair model

We introduce the d-dimensional analog of the Dilcher–Girstmair model. We begin gently with the two-dimensional extension: Given three positive integers a, b, and c, divide one of the sides of the square $[0,a)\times[0,a)$ into b parts of length a/b, and the other side into c parts of length a/c. This division induces a grid (see Fig. 1 for an example). We thus have bc boxes of equal size. We think of each box as half open: We count the left (excluding the highest point) and bottom side (excluding the right-most point) as belonging to the box. Let us mark each box by a pair of integers (j,k) where $0\leqslant j\leqslant b-1$ and $0\leqslant k\leqslant c-1$. We will study the integer lattice points in the square $[0,a)\times[0,a)$; note that the box (j,k) contains the point $(m,n)\in\mathbb{Z}^2$ if and only if

$$\frac{ja}{b}\leqslant m<\frac{(j+1)a}{b}\quad\text{and}\quad\frac{ka}{c}\leqslant n<\frac{(k+1)a}{c}. \tag{2.1}$$

Equivalent to this condition is the following condition:

$$j\leqslant\frac{mb}{a}<j+1\quad\text{and}\quad k\leqslant\frac{nc}{a}<k+1,$$

which can be rewritten in compact form using the greatest integer function $\lfloor x\rfloor$ (the greatest integer not exceeding x):

$$j=\left\lfloor\frac{mb}{a}\right\rfloor\quad\text{and}\quad k=\left\lfloor\frac{nc}{a}\right\rfloor. \tag{2.2}$$

We formalize the distribution of integer points within each of the bc boxes as follows.

Definition 1. Let $f_{a;b,c}(j,k)$ denote the number of diagonal lattice points in the box (j,k).

Notice that most of these frequencies are zero. We can evaluate the following sum in two ways according to the equivalence of (2.1) and (2.2):

$$\sum_{j=0}^{b-1}\sum_{k=0}^{c-1}jkf_{a;b,c}(j,k)=\sum_{m=0}^{a-1}\left\lfloor\frac{mb}{a}\right\rfloor\left\lfloor\frac{mc}{a}\right\rfloor. \tag{2.3}$$

A special case of this equality is $b=c$, for which we make the following definition.

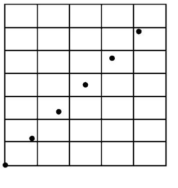

Fig. 1. $a=6$, $b=5$, $c=7$.

Definition 2. Let $f_{a;b}(j)$ denote the number of integers in the jth subinterval when we divide $[0,a)$ into b equal parts.

We remark that when $b=c$, we trivially get $f_{a;b,c}(j)=f_{a;b}(j)$. Furthermore, the condition $b=c$ implies that the b boxes on the diagonal of the cube cover the diagonal completely—in the sense that no other (j,k) box contains lattice points on the diagonal. Thus, for $b=c$, and any $j\neq k$, we have

$$f_{a;b,c}(j,k)=0.$$

We conclude that when $b=c$ the double sums reduce to the one-dimensional sums studied by Dilcher and Girstmair, i.e.

$$\sum_{j=0}^{b-1}\sum_{k=0}^{b-1} jk f_{a;b,b}(j,k)=\sum_{j=0}^{b-1} j^2 f_{a;b}(j)=\sum_{m=0}^{a-1}\left\lfloor \frac{mb}{a}\right\rfloor^2. \tag{2.4}$$

The sum on the right hand is essentially a classical Dedekind sum: If a and b are relatively prime,

$$\begin{aligned}
\sum_{m=0}^{a-1}\left\lfloor \frac{mb}{a}\right\rfloor^2 &= \sum_{m=1}^{a-1}\left(\frac{mb}{a}-\left\{\frac{mb}{a}\right\}\right)^2\\
&= \sum_{m=1}^{a-1}\left(\frac{mb}{a}\right)^2-2\sum_{m=1}^{a-1}\frac{mb}{a}\left\{\frac{mb}{a}\right\}+\sum_{m=1}^{a-1}\left\{\frac{mb}{a}\right\}^2\\
&= \frac{b^2}{a^2}\sum_{m=1}^{a-1} m^2-2b\sum_{m=1}^{a-1}\left(\frac{m}{a}-\frac{1}{2}\right)\left(\left\{\frac{mb}{a}\right\}-\frac{1}{2}\right)\\
&\quad -2b\sum_{m=1}^{a-1}\frac{m}{a}+\frac{2b(a-1)}{4}+\sum_{m=1}^{a-1}\left(\frac{m}{a}\right)^2\\
&= \frac{(b^2+1)(a-1)(2a-1)}{6a}-2bs(b,a)-\frac{1}{2}b(a-1).
\end{aligned}$$

This and similar sums coming from the one-dimensional case will appear repeatedly in the exposition that follows.

Definition 3. For any two positive integers a and b, let

$$M_k(a;b)=\frac{1}{a}\sum_{m=0}^{a-1}\left\lfloor \frac{mb}{a}\right\rfloor^k.$$

M_k is the kth moment of the Dilcher–Girstmair probability distribution (see Section 6). By (2.4), and by an argument identical to the one that preceded (2.4), now applied to the diagonal lattice points of the k-dimensional cube, the definition of M_k is equivalent to

$$M_k(a;b) = \frac{1}{a}\sum_{j=0}^{b-1} j^k f_{a;b}(j).$$

We just showed above that M_2 corresponds to the classical Dedekind sum $s(a,b)$ as in (1.5).

The model that we described above extends naturally to higher dimensions. Instead of considering a square, we divide the d-dimensional cube $[0,a) \times \cdots \times [0,a)$ into $b_1 \cdots b_d$ equal boxes by a similar construction as above: Now we divide the first side into b_1 equal intervals, the next one into b_2 equal intervals, and so on. Again we will count the number of diagonal integer lattice points of this cube, according to the box they are in. As above we will label each box by $(k_1,\dots,k_d)$, with $0 \leqslant k_j \leqslant b_j - 1$, and we will denote the function counting the lattice points in box $(k_1,\dots,k_d)$ by

$$f_{a;b_1,\dots,b_d}(k_1,\dots,k_d).$$

As before, an elementary counting-two-ways argument yields

$$\sum_{k_1=0}^{b_1-1}\cdots\sum_{k_d=0}^{b_d-1} k_1\cdots k_d\, f_{a;b_1,\dots,b_d}(k_1,\dots,k_d) = \sum_{m=0}^{a-1}\left\lfloor\frac{mb_1}{a}\right\rfloor\cdots\left\lfloor\frac{mb_d}{a}\right\rfloor.$$

This naturally leads to the following definition.

Definition 4. For positive integers $a, b_1, b_2, \dots, b_d$, we define

$$S_d(a;\mathbf{b}) = S_d(a;b_1,b_2,\dots,b_d) = \frac{1}{a}\sum_{m=0}^{a-1}\left\lfloor\frac{mb_1}{a}\right\rfloor\cdots\left\lfloor\frac{mb_d}{a}\right\rfloor.$$

This is a generalized Dedekind sum. Our goal is to find relations for the sums $S_d(a;\mathbf{b})$, using statistical methods.

3. The two-dimensional frequency distribution $\{f_{a;b,c}(j,k)\}$ and its marginal distributions

In this section we focus on the study of the distribution frequencies $f_{a;b,c}(j,k)$ using the duality interpretation given by (2.3). As we lack a closed formula for the number of diagonal lattice points that belong to the (j,k)th box (that is, for $f_{a;b,c}(j,k)$, $j = 0,\dots,b-1$,

Table 1
The two-dimensional distribution and its marginals for $a = 50$, $b = 13$, $c = 7$

$j \setminus k$	0	1	2	3	4	5	6	$f^a_b(j)$
0	4	0	0	0	0	0	0	4
1	4	0	0	0	0	0	0	4
2	0	4	0	0	0	0	0	4
3	0	3	1	0	0	0	0	4
4	0	0	4	0	0	0	0	4
5	0	0	2	2	0	0	0	4
6	0	0	0	3	0	0	0	3
7	0	0	0	2	2	0	0	4
8	0	0	0	0	4	0	0	4
9	0	0	0	0	1	3	0	4
10	0	0	0	0	0	4	0	4
11	0	0	0	0	0	0	4	4
12	0	0	0	0	0	0	3	3
$f^a_c(k)$	8	7	7	7	7	7	7	50

$k = 0, \dots, c-1$) we developed an algorithm, given in the appendix, for computing the values of $f_{a;b,c}(j,k)$ and of the marginal frequencies

$$f_{a;b}(j) = \sum_{k=0}^{c-1} f_{a;b,c}(j,k) \quad \text{and} \quad f_{a;c}(k) = \sum_{j=0}^{b-1} f_{a;b,c}(j,k).$$

We note that these marginal frequencies are not new objects, and coincide with their lower-dimensional brethren.

Example. In Table 1 we present these distributions for the case $a = 50$, $b = 13$, $c = 7$. From this table we can immediately verify that

$$\sum_{j=0}^{12} \sum_{k=0}^{6} kj f_{50;13,7}(j,k) = \sum_{m=0}^{49} \left\lfloor \frac{13m}{50} \right\rfloor \left\lfloor \frac{7m}{50} \right\rfloor = 1236.$$

By analyzing the structure of the marginal distributions we can arrive at closed formulae for $M_k(a;b)$. For example, one can immediately verify that

$$f_{a;b}(j) = n = \frac{a}{b}, \quad j = 0, \dots, b-1, \quad \text{if } a \equiv 0 \bmod b,$$

and

$$f_{a;b}(j) = \begin{cases} \left\lfloor \frac{a}{b} \right\rfloor + 1, & \text{if } j = 0, \\ \left\lfloor \frac{a}{b} \right\rfloor, & \text{if } j > 0, \end{cases} \qquad \text{if } a \equiv 1 \bmod b. \tag{3.1}$$

Thus for $a \equiv 0, 1 \mod b$ we immediately obtain

$$M_k(a;b) = \frac{1}{a}\left\lfloor \frac{a}{b} \right\rfloor \sum_{j=1}^{b-1} j^k.$$

In general, the one-dimensional frequencies can be bounded as

$$\left\lfloor \frac{a}{b} \right\rfloor \leqslant f_{a;b}(j) < \left\lceil \frac{a}{b} \right\rceil. \tag{3.2}$$

A book-keeping device that will help us keep track of the difference between the frequency $f_{a;b}(j)$ and $\lfloor a/b \rfloor$ is the following.

Definition 5. $I_{a;b}(j) = f_{a;b}(j) - \lfloor a/b \rfloor$.

Notice that by (3.2) we have $I_{a;b}(j) \in \{0, 1\}$ for all a, b and for all $j \in \{0, \ldots, b-1\}$. Accordingly we rewrite the kth moment of the Dilcher–Girstmair distribution as follows:

$$M_k(a;b) = \frac{1}{a}\left(\left\lfloor \frac{a}{b} \right\rfloor \sum_{j=1}^{b-1} j^k + \sum_{j=1}^{b-1} j^k I_{a;b}(j)\right). \tag{3.3}$$

The second sum allows for a finer analysis of these moments. A trivial example follows from the fact that $I_{a;b}(j) \geqslant 0$:

$$M_k(a;b) \geqslant \frac{1}{a}\left\lfloor \frac{a}{b} \right\rfloor \sum_{j=1}^{b-1} j^k.$$

This bound gets achieved, for example, when $a \equiv 0, 1 \mod b$. In the following section, we study $I_{a;b}(j)$ and its second moments.

4. Some formulae and bounds for M_2

Of special interest is $M_2(a;b)$, due to its relationship to the Dedekind sum $s(a,b)$. According to (3.3) we have

$$aM_2(a;b) = \left\lfloor \frac{a}{b} \right\rfloor \frac{(b-1)b(2b-1)}{6} + \sum_{j=1}^{b-1} j^2 I_{a;b}(j). \tag{4.1}$$

One may think about this identity in terms of the Dilcher–Girstmair distribution model: Among the a integers in $[0, a)$, we have at least $\lfloor a/b \rfloor$ of them in each interval

$$\left[\frac{ka}{b}, \frac{(k+1)a}{b}\right), \quad k = 0, \ldots, b-1.$$

These integers are represented in the first term on the right-hand side of (4.1). Suppose $a \equiv l \mod b$ where $0 < l < b$ (the case $b \mid a$ is special and very easy to handle: $I_{a;b}(j) = 0$ for all j); then there are $l - 1$ integers "left" which haven't been accounted for (note that the first interval $[0, a/b)$ contains $\lfloor a/b \rfloor + 1$ integers). These $l - 1$ integers are represented in the second term on the right-hand side of (4.1). In fact, one can say more about them. Because they are uniformly distributed among the b intervals, we obtain

$$D_2(a; b) = \sum_{j=1}^{b-1} j^2 I_{a;b}(j) = \sum_{m=1}^{l-1} \left\lfloor \frac{mb}{l} \right\rfloor^2 = l M_2(l; b), \quad l \geqslant 2. \tag{4.2}$$

Note that, in particular, $D_2(a; b)$ depends on a only via $l \equiv a \mod b$. For special values of $a \equiv l \mod b$, we can obtain closed formulas for $D_2(a; b)$, given in the following theorem.

Theorem 1. *Let $l \equiv a \mod b$. Then $D_2(a; b)$ is given by the following formulae*:

l	$D_2(a; b)$	
0, 1	0	
2	$\lfloor \frac{b}{2} \rfloor^2$	
3	$5\lfloor \frac{b}{3} \rfloor^2$	if $b \equiv 0, 1 \mod 3$
	$5\lfloor \frac{b}{3} \rfloor^2 + 4\lfloor \frac{b}{3} \rfloor + 1$	if $b \equiv 2 \mod 3$
4	$14\lfloor \frac{b}{4} \rfloor^2$	if $b \equiv 0, 1 \mod 4$
	$14\lfloor \frac{b}{4} \rfloor^2 + 10\lfloor \frac{b}{4} \rfloor + 2$	if $b \equiv 2 \mod 4$
	$14\lfloor \frac{b}{4} \rfloor^2 + 16\lfloor \frac{b}{4} \rfloor + 5$	if $b \equiv 3 \mod 4$
5	$30\lfloor \frac{b}{5} \rfloor^2$	if $b \equiv 0, 1 \mod 5$
	$30\lfloor \frac{b}{5} \rfloor^2 + 14\lfloor \frac{b}{5} \rfloor + 2$	if $b \equiv 2 \mod 5$
	$30\lfloor \frac{b}{5} \rfloor^2 + 26\lfloor \frac{b}{5} \rfloor + 6$	if $b \equiv 3 \mod 5$
	$30\lfloor \frac{b}{5} \rfloor^2 + 40\lfloor \frac{b}{5} \rfloor + 14$	if $b \equiv 4 \mod 5$

Proof. This table follows directly from (4.2). □

To illustrate one typical case, let $l = 3$. In this case $D_2(a; b) = \lfloor b/3 \rfloor^2 + \lfloor 2b/3 \rfloor^2$, by definition. When $b \equiv 0 \mod 3$, so that $b = 3n$, the expression $D_2(a; b)$ simplifies to $\lfloor n \rfloor^2 + \lfloor 2n \rfloor^2 = 5n^2$. In the case that $b \equiv 1 \mod 3$, so that $b = 3n + 1$, we get

$$D_2(a; b) = \left\lfloor n + \frac{1}{3} \right\rfloor^2 + \left\lfloor 2n + \frac{4}{3} \right\rfloor^2 = n^2 + (2n + 1)^2 = 5n^2 + 4n + 1,$$

verifying the third entry in the table.

In general, one can use (4.2) to obtain inequalities for $D_2(a;b)$ and hence for $M_2(a;b)$. To this end, we use the fact that

$$\left(m\left\lfloor\frac{b}{l}\right\rfloor\right)^2 \leqslant \left\lfloor\frac{mb}{l}\right\rfloor^2 \leqslant \left\lfloor\left(\frac{mb}{l}\right)\right\rfloor^2, \quad l \geqslant 1,$$

which implies the following bounds for $l \geqslant 2$:

$$\left\lfloor\frac{b}{l}\right\rfloor^2 \sum_{m=1}^{l-1} m^2 = \left\lfloor\frac{b}{l}\right\rfloor^2 \frac{(l-1)l(2l-1)}{6} \leqslant D_2(a;b) \leqslant \left\lfloor\left(\frac{b}{l}\right)^2 \frac{(l-1)l(2l-1)}{6}\right\rfloor$$
$$= \left\lfloor\sum_{m=1}^{l-1}\left(\frac{mb}{l}\right)^2\right\rfloor.$$

Accordingly, we have the following:

Theorem 2. *For* $a \equiv l \mod b$

$$aM_2(a;b) = \left\lfloor\frac{a}{b}\right\rfloor \frac{(b-1)b(2b-1)}{6}, \quad \textit{if } l = 0, 1, \tag{4.3}$$

and for $l \geqslant 2$

$$aM_2(a;b) \geqslant \left\lfloor\frac{a}{b}\right\rfloor \frac{(b-1)b(2b-1)}{6} + \left\lfloor\frac{b}{l}\right\rfloor^2 \frac{(l-1)l(2l-1)}{6} \tag{4.4}$$

and

$$aM_2(a;b) \leqslant \left\lfloor\frac{a}{b}\right\rfloor \frac{(b-1)b(2b-1)}{6} + \left\lfloor\frac{b^2(l-1)(2l-1)}{6l}\right\rfloor. \tag{4.5}$$

Naturally, $D_2(a;b)$ can be approximated further to give even better bounds. We illustrate one further step here. Suppose as before that $a \equiv l \mod b$ where $1 < l < b$, and moreover that $b \equiv k \mod l$, so that $b = \lfloor b/l \rfloor l + k$, with $0 \leqslant k \leqslant l-1$. According to (4.2) this congruence restriction gives

$$D_2(a;b) = \sum_{m=1}^{l-1}\left\lfloor\frac{mb}{l}\right\rfloor^2 = \sum_{m=1}^{l-1}\left\lfloor\frac{m(\lfloor b/l\rfloor l + k)}{l}\right\rfloor^2 = \sum_{m=1}^{l-1}\left(m\left\lfloor\frac{b}{l}\right\rfloor + \left\lfloor\frac{mk}{l}\right\rfloor\right)^2$$
$$= \left\lfloor\frac{b}{l}\right\rfloor^2 \frac{(l-1)l(2l-1)}{6} + 2\left\lfloor\frac{b}{l}\right\rfloor \sum_{m=1}^{l-1} m\left\lfloor\frac{mk}{l}\right\rfloor + \sum_{m=1}^{l-1}\left\lfloor\frac{mk}{l}\right\rfloor^2.$$

Lemma 3. *For all $l \geqslant 2$*

$$D_2(a;b) = \left\lfloor \frac{b}{l} \right\rfloor^2 \frac{(l-1)l(2l-1)}{6}, \quad \textit{if } k = 0 \textit{ or } 1,$$

$$D_2(a;b) = \left\lfloor \frac{b}{l} \right\rfloor^2 \frac{(l-1)l(2l-1)}{6} + \begin{cases} \lfloor \frac{b}{l} \rfloor \big((l-1)l - \frac{1}{4}l(l-2)\big) + \frac{l}{2}, & \textit{if } l \textit{ is even}, \\ \lfloor \frac{b}{l} \rfloor (l-1)l - \lfloor \frac{l}{2} \rfloor \big(1 + \lfloor \frac{l}{2} \rfloor\big) + \lfloor \frac{l}{2} \rfloor, & \textit{if } l \textit{ is odd}, \end{cases} \tag{4.6}$$

if $k = 2$.

For example, if $l = 4$, $k = 2$

$$D_2(4,b) = \left\lfloor \frac{b}{4} \right\rfloor^2 \frac{3 \cdot 4 \cdot 7}{6} + 10 \left\lfloor \frac{b}{4} \right\rfloor + 2,$$

and if $l = 5$, $k = 2$

$$D_2(5,b) = \left\lfloor \frac{b}{5} \right\rfloor^2 \frac{4 \cdot 5 \cdot 9}{6} + 14 \left\lfloor \frac{b}{5} \right\rfloor + 2,$$

as stated in Theorem 1. Finally, since $\lfloor mk/l \rfloor \geqslant \lfloor m2/l \rfloor$ for all $k \geqslant 2$, the above formula for $D_2(a;b)$ with $k = 2$ is a lower bound.

Similar bounds can be derived "classically" by applying Dedekind's famous reciprocity law:

Theorem 4 (Dedekind). *If a and b are relatively prime then*

$$s(a,b) + s(b,a) = -\frac{1}{4} + \frac{1}{12}\left(\frac{a}{b} + \frac{1}{ab} + \frac{b}{a}\right). \tag{4.7}$$

Denote the rational function appearing in Theorem 4 by

$$R(a,b) = -\frac{1}{4} + \frac{1}{12}\left(\frac{a}{b} + \frac{1}{ab} + \frac{b}{a}\right). \tag{4.8}$$

Then we obtain for $a \equiv l \mod b$, where a and b are relatively prime and $1 < l < b$,

$$s(b,a) = R(a,b) - s(a,b) = R(a,b) - s(l,b) = R(a,b) - R(b,l) + s(b,l).$$

It is an easy exercise (see the Carus monograph *Dedekind Sums* by Rademacher and Grosswald) that

$$\left|s(b,l)\right| \leqslant s(1,l) = \frac{l}{12} - \frac{1}{4} + \frac{1}{6l}, \tag{4.9}$$

which gives the following bounds:

$$R(a,b) - R(b,l) - s(1,l) \leqslant s(b,a) \leqslant R(a,b) - R(b,l) + s(1,l). \tag{4.10}$$

These inequalities, in turn, can be transformed into inequalities for M_2 via (1.5), to obtain:

Theorem 5. *Lower and upper bounds for M_2 are*:

$$\begin{aligned} M_2(a;b) \geqslant{} & \frac{(b^2+1)(a-1)(2a-1)}{6a^2} - \frac{(a-1)b}{2a} \\ & - \frac{2b}{a}\big(R(a,b) - R(b,l) + s(1,l)\big), \end{aligned} \tag{4.11}$$

$$\begin{aligned} M_2(a;b) \leqslant{} & \frac{(b^2+1)(a-1)(2a-1)}{6a^2} - \frac{(a-1)b}{2a} \\ & - \frac{2b}{a}\big(R(a,b) - R(b,l) - s(1,l)\big). \end{aligned} \tag{4.12}$$

In Table 2 we give the exact values of $aM_2(a;b)$ and their lower bounds. We denote by

flb1	the lower bound according to (4.4),
flb2	the lower bound according to (4.6),
rlb	the lower bound according to (4.11),
fub	the upper bound according to (4.5),
rub	the upper bound according to (4.12).

Note that we can compute rlb and rub only when a and b are relatively prime.

5. Bounds for generalized Dedekind sums: The case $d = 2$

5.1. Applications of the Cauchy–Schwartz inequality

In the present section we discuss some relationships between the S and the M-functions. By definition, if $b_1 = \cdots = b_d$

$$S_d(a; b\,\mathbf{1}_d) = M_d(a;b), \quad d = 1, 2, \ldots.$$

Table 2

a	b	exact	flb1	flb2	rlb	fub	rub
5	2	2	2	2	2	2	2
5	3	6	6	6	6	6	6
5	4	14	14	14	14	14	14
6	2	3	3	3		3	
6	3	10	10	10		10	
6	4	18	18	18		18	
6	5	30	30	30	30	30	30
7	2	3	3	3	3	3	3
7	3	10	10	10	10	10	10
7	4	19	19	19	19	19	19.9
7	5	34	34	34	34	34	34
7	6	55	55	55	55	55	55
35	7	455	455	455		455	
39	7	490	469	481	486.5	497	490
40	7	501	485	501	498.2	513	503.8
41	7	510	510	510	510	529	517.8
10	3	15	15	15	15	15	15
11	3	16	16	16	16	16	16
21	6	185	185	185		185	
20	6	174	174	174		174	
11	7	126	105	117	122.5	133	126
10	9	204	204	204	204	204	204
11	9	220	220	220	220	220	220
12	9	249	249	249		249	
13	9	260	260	260	260	274	264.5
14	9	288	234	250	280.8	301	288
15	9	315	259	286		327	
16	9	328	295	328	322.9	354	335.7
17	9	344	344	344	344	381	359.75
24	10	648	626	648		657	

Here $\mathbf{1}_d$ denotes the d-dimensional vector all of whose components are 1. The Cauchy–Schwartz inequality yields immediately, for $d = 2$, the inequality

$$S_2(a; b_1, b_2) \leqslant \big(M_2(a; b_1)M_2(a; b_2)\big)^{1/2},$$

with equality if and only if $b_1 = b_2$. Let

$$R_2(a; b_1, b_2) = \frac{S_2(a; b_1, b_2)}{\sqrt{M_2(a; b_1)M_2(a; b_2)}}. \tag{5.1}$$

In Table 3 we give a few values of $R_2(a; b_1, b_2)$.

It is interesting to observe in this table that all these $R_2(a; b, c)$-values are close to 1, and that among these values $R_2(a; 2, b_2) < R_2(a; 3, b_2)$. The question is whether this inequality is always true. A partial answer is given in Lemma 10 of Section 5.2. Empirical evaluations lead us to the following conjecture:

Table 3

a	b_2	$R_2(a;2,b_2)$	$R_2(a;3,b_2)$
11	7	0.9163	0.9799
21	5	0.9237	0.9721
18	11	0.9297	0.9729
73	39	0.9189	0.9695
99	33	0.9192	0.9707

Conjecture 1. *For all* $a, b, c \geqslant 3$,

$$R_2(a;b,c) \geqslant R_2(5;2,3) = \frac{\sqrt{3}}{2}. \tag{5.2}$$

Notice that according to the previous definitions, $R_2(a;b,c)$ is the cosine of the angle between the two vectors

$$\mathbf{v}_b = \left(\left\lfloor \frac{b}{a} \right\rfloor, \left\lfloor \frac{2b}{a} \right\rfloor, \ldots, \left\lfloor \frac{(a-1)b}{a} \right\rfloor\right) \quad \text{and} \quad \mathbf{v}_c = \left(\left\lfloor \frac{c}{a} \right\rfloor, \left\lfloor \frac{2c}{a} \right\rfloor, \ldots, \left\lfloor \frac{(a-1)c}{a} \right\rfloor\right).$$

In Section 5.2 we present the geometrical correspondence, which is utilized to obtain further results.

Exact formulae can be derived for $R_2(a;2,a)$, $a \geqslant 3$. Indeed

$$S_2(a;2,a) = \begin{cases} \frac{a-1}{2} - \frac{\lfloor a/2 \rfloor (1+\lfloor a/2 \rfloor)}{2a}, & \text{if } \left\lfloor \frac{a}{2} \right\rfloor < \frac{a}{2}, \text{ i.e. } a \text{ is odd}, \\ \frac{a-1}{2} - \frac{1}{4}\left(\frac{a}{2} - 1\right), & \text{if } \left\lfloor \frac{a}{2} \right\rfloor = \frac{a}{2}, \text{ i.e. } a \text{ is even}. \end{cases} \tag{5.3}$$

Moreover

$$M_2(a;2) = \frac{1}{a} \left\lfloor \frac{a}{2} \right\rfloor$$

and

$$M_2(a;a) = \frac{2a^2 - 3a + 1}{6}.$$

Accordingly

$$R_2(a;2,a) = \begin{cases} R_2^*(a)\left(a - 1 - \frac{\lfloor a/2 \rfloor (1+\lfloor a/2 \rfloor)}{a}\right), & \text{if } \left\lfloor \frac{a}{2} \right\rfloor < \frac{a}{2}, \text{ i.e. } a \text{ is odd}, \\ R_2^*(a)\left(a - 1 - \frac{a/2-1}{2}\right), & \text{if } \left\lfloor \frac{a}{2} \right\rfloor = \frac{a}{2}, \text{ i.e. } a \text{ is even}, \end{cases} \tag{5.4}$$

where

$$R_2^*(a) = \frac{\sqrt{6a}}{2\sqrt{\lfloor a/2 \rfloor (2a^2 - 3a + 1)}}. \tag{5.5}$$

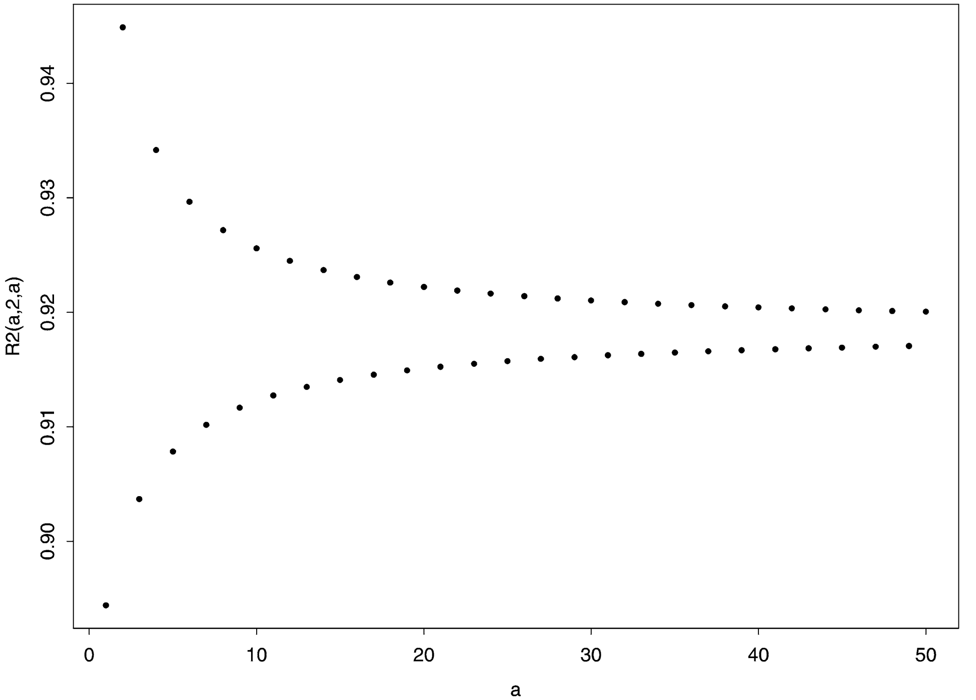

Fig. 2. $R_2(a;2,a)$ for $a=3,\dots,50$.

A graph of $R_2(a;2,a)$ for $a=3,\dots,50$ is given in Fig. 2. Notice that $\lim_{a\to\infty} R_2(a;2,a)=3\sqrt{6}/8$.

We provide here a few auxiliary results. First, if $c=l+ia$ (i.e. $a\equiv l \bmod c$) then

$$S_2(a;b,c)=\sum_{m=0}^{a-1}\left\lfloor\frac{bm}{a}\right\rfloor\left\lfloor\frac{(l+ia)m}{a}\right\rfloor=i\sum_{m=1}^{a-1}m\left\lfloor\frac{bm}{a}\right\rfloor+S_2(a;b,l). \tag{5.6}$$

Similarly,

$$aM_2(a;l+ia)=\sum_{m=0}^{a-1}\left\lfloor\frac{(l+ia)m}{a}\right\rfloor^2=i^2\frac{(a-1)a(2a-1)}{6}+2i\sum_{m=1}^{a-1}m\left\lfloor\frac{lm}{a}\right\rfloor + aM_2(a,l).$$

Accordingly,

$$R_2(a;b,l+ia)=\frac{i\sum_{m=1}^{a-1}m\lfloor\frac{bm}{a}\rfloor+aS_2(a;b,l)}{D_i} \tag{5.7}$$

where

$$D_i = i\left(aM_2(a;b)\frac{(a-1)a(2a-1)}{6} + \frac{2}{i}\sum_{m=1}^{a-1} m\left\lfloor\frac{lm}{a}\right\rfloor + \frac{a}{i^2}M_2(a,l)\right)^{1/2}.$$

Thus,

$$\lim_{c\to\infty} R_2(a;b,c) = \lim_{i\to\infty} R_2(a;b,l+ia) = R_2(a;b,a).$$

Now,

$$aS_2(a;ja,a) = \sum_{m=0}^{a-1}\left\lfloor\frac{mja}{a}\right\rfloor\left\lfloor\frac{ma}{a}\right\rfloor = j\sum_{m=0}^{a-1} m^2 = j\frac{(a-1)a(2a-1)}{6}$$

and

$$aM_2(a;ja) = j^2\sum_{m=0}^{a-1} m^2 = j^2\frac{(a-1)a(2a-1)}{6},$$

whence

$$R_2(a;ja,a) = 1 \quad \text{for all } j \geqslant 1.$$

We consider now $R_2(a;b,a)$ with $a\to\infty$. Let $a = jb$. For $j \geqslant 2$

$$R_2(jb;b,jb) = \frac{\sum_{m=j}^{jb-1} m\lfloor\frac{m}{j}\rfloor}{\left(\sum_{m=j}^{jb-1}\lfloor\frac{m}{j}\rfloor^2\frac{(a-1)a(2a-1)}{6}\right)^{1/2}},$$

$$\sum_{m=j}^{jb-1} m\left\lfloor\frac{m}{j}\right\rfloor = \sum_{l=1}^{b-1} l\sum_{m=lj}^{(l+1)j-1} m = \frac{bj(b-1)(4bj+j-3)}{12},$$

$$\sum_{m=j}^{jb-1}\left\lfloor\frac{m}{j}\right\rfloor^2 = j\sum_{l=1}^{b-1} l^2 = j\frac{(b-1)b(2b-1)}{6}.$$

Thus

$$\begin{aligned} R_2^*(b) &= \lim_{j\to\infty} R_2(jb;b,jb) = \lim_{j\to\infty}\frac{(b-1)((4b+1)j-3)}{2((b-1)(2b-1)(jb-1)(2jb-1))^{1/2}} \\ &= \frac{\sqrt{2}(b-1)(4b+1)}{4b\sqrt{(b-1)(2b-1)}}. \end{aligned} \tag{5.8}$$

Some values of the limit are given in Table 4.

Table 4
Some values of $R_2^*(b) = \lim_{j\to\infty} R_2(jb; b, jb)$

b	$R_2^*(b)$
2	0.918558
3	0.96896
4	0.9836

5.2. *A geometric correspondence*

We have seen that the Dedekind-like sums $S_2(a; b, c)$ and $M_2(a; b)$ can be considered as inner products in $\mathbb{R}^{a-1}$. Thus, for a given integer $a \geqslant 3$, we construct a polyhedral cone $\mathcal{C}_a \subset \mathbb{R}^{a-1}$ that is defined by the positive real span of the vectors

$$\mathbf{v}_b = \left(\left\lfloor \frac{b}{a} \right\rfloor, \left\lfloor \frac{2b}{a} \right\rfloor, \dots, \left\lfloor \frac{(a-1)b}{a} \right\rfloor\right), \quad 1 \leqslant b < \infty.$$

As stated in the introduction, the significance of these vectors is that $R_2(a; b, c)$ is the cosine of the angle between the two vectors $\mathbf{v}_b$ and $\mathbf{v}_c$. The observation that $R_2(a; b, c)$ is close to 1 is captured geometrically by the statement that this cone $\mathcal{C}_a$ is thin in the angular metric.

Notice that $\mathbf{v}_1 = \mathbf{0} = (0, \dots, 0)$ and $\mathbf{v}_a = (1, 2, \dots, a-1)$. For $b = 2, 3, \dots, a-1$, the vectors $\mathbf{v}_b$ are

$$\begin{aligned}
&\mathbf{v}_2 = (0, \dots, 0, 1, \dots, 1), \quad \mathbf{v}_3 = (0, \dots, 0, 1, \dots, 1, 2, \dots, 2), \quad \dots, \\
&\mathbf{v}_{a-1} = (0, 1, \dots, a-2),
\end{aligned}$$

where each vector $\mathbf{v}_j$ has almost equally distributed values for the integers the comprise its entries.

For $b > a$, we write $b = ka + l$, $k > 0$, $0 \leqslant l < a$, and it follows from our notation that $\mathbf{v}_b = k\mathbf{v}_a + \mathbf{v}_l$. Thus the cone $\mathcal{C}_a$ is in fact the positive real span of only the $a-1$ vectors $\mathbf{v}_b$ with $b = 2, 3, \dots, a$.

Since $\mathbf{v}_1 = 0$, we have $\mathbf{v}_{ka} = \mathbf{v}_{ka+1}$. Moreover, if P_l $(2 \leqslant l \leqslant a-1)$ denotes the 2-dimensional plane containing the vectors $\mathbf{v}_l$ and $\mathbf{v}_a$, then all the vectors $\mathbf{v}_{ka+l}$, $k = 0, 1, \dots,$ belong to P_l. Notice that for different values of l, say l and $l' \neq l$, P_l and $P_{l'}$ are two different planes which have the ray

$$\{r\mathbf{v}_a\colon\, r \geqslant 0\}$$

in common (see Lemma 6). Throughout this section, the denominators in the vector components of all the vectors $\mathbf{v}_m$ are always the same integer a.

The vectors $\mathbf{v}_2, \dots, \mathbf{v}_a$ are not always linearly independent. One can easily check that if $a = 3, 4, 6$ then these vectors are linearly independent, and when $a = 5, 7, 8, 9, \dots$ they are not. However, one can prove the following:

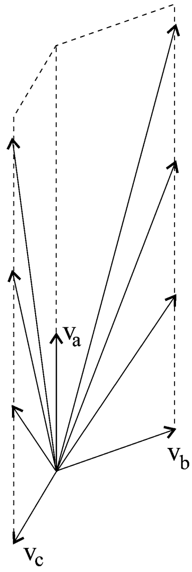

Fig. 3. $\mathbf{v}_a$, $\mathbf{v}_b + k\mathbf{v}_a$ $(0 \leqslant k \leqslant 3)$, $\mathbf{v}_c + j\mathbf{v}_a$ $(0 \leqslant j \leqslant 3)$.

Lemma 6. *For each $a \geqslant 4$, the vectors $\mathbf{v}_a, \mathbf{v}_l, \mathbf{v}_{l'}$, where $1 < l, l' < a$ and $l \neq l'$, are linearly independent.*

Proof. For each $a \geqslant 4$, $\mathbf{v}_a = (1, 2, \dots, a-1)$, while the first component of both $\mathbf{v}_l$ and $\mathbf{v}_{l'}$ is zero; thus $\mathbf{v}_a$ is linearly independent of $\{\mathbf{v}_l, \mathbf{v}_{l'}\}$. Moreover, $\mathbf{v}_l$ and $\mathbf{v}_{l'}$ do not lie on the same ray. $\square$

Lemma 7. *For each $a \geqslant 3$, if $b_1 = k_1 a + l$ and $b_2 = k_2 a + l$, where $1 \leqslant k_1 < k_2$, then*

$$R_2(a; l, a) < R_2(a; l, b_2) < R_2(a; l, b_1)$$

for all $1 < l < a$.

Proof. The vectors $\mathbf{v}_{b_1}$ and $\mathbf{v}_{b_2}$ lie in P_l. Moreover, $\mathbf{v}_{b_1} = k_1\mathbf{v}_a + \mathbf{v}_l$ and $\mathbf{v}_{b_2} = k_2\mathbf{v}_a + \mathbf{v}_l$. Hence

$$\angle(\mathbf{v}_l, \mathbf{v}_a) > \angle(\mathbf{v}_{b_1}, \mathbf{v}_a) > \angle(\mathbf{v}_{b_1}, \mathbf{v}_a).$$

But $\angle(\mathbf{v}_b, \mathbf{v}_l) = \angle(\mathbf{v}_a, \mathbf{v}_l) - \angle(\mathbf{v}_a, \mathbf{v}_b)$, and the inequalities in the statement follow by taking cosines. $\square$

Notice that due to the monotonicity stated in the last lemma,

$$\lim_{k\to\infty} R_2(a; l, ka + l) = R_2(a; l, a).$$

It is interesting to notice that in the case of $a = 3$, all vectors $\mathbf{v}_b$ are between $\mathbf{v}_2 = (0, 1)$ and $\mathbf{v}_3 = (1, 2)$. The cosine of the angle between these two vectors is $2/\sqrt{5}$.

Lemma 8.

(i) *If $a = 3, 5$ then $R_2(a; 2, b) < R_2(a; 3, b)$ for all $b \geqslant 3$.*
(ii) *If $a = 4$ then $R_2(4; 2, b) < R_2(4; 3, b)$ for all $b \neq 6$. If $b = 6$ then $R_2(4; 2, 6) = 0.9708$ and $R_2(4; 3, 6) = 0.9647$.*

Proof. (i) The case $a = 3$ follows immediately from Lemma 7. For $a = 5$ we have

$$\begin{aligned} \mathbf{v}_2 &= (0, 0, 1, 1), & |\mathbf{v}_2| &= \sqrt{2}, \\ \mathbf{v}_3 &= (0, 1, 1, 2), & |\mathbf{v}_3| &= \sqrt{6}, \\ \mathbf{v}_4 &= (0, 1, 2, 3), & |\mathbf{v}_4| &= \sqrt{14}, \\ \mathbf{v}_5 &= (1, 2, 3, 4), & |\mathbf{v}_5| &= \sqrt{30}. \end{aligned}$$

Let $(\cdot,\cdot)$ denote the inner product of two vectors. For any $b = 5k + l$, $k = 1, 2, \ldots,$ $l = 2, 3, 4$,

$$R_2(5; 2, 5k + l) < R_2(5; 3, 5k + l)$$

if and only if

$$\frac{1}{\sqrt{2}}(\mathbf{v}_2, \mathbf{v}_{5k+l}) < \frac{1}{\sqrt{6}}(\mathbf{v}_3, \mathbf{v}_{5k+l}).$$

This is equivalent to

$$\sqrt{6}k(\mathbf{v}_2, \mathbf{v}_5) + \sqrt{6}(\mathbf{v}_2, \mathbf{v}_l) < \sqrt{2}k(\mathbf{v}_3, \mathbf{v}_5) + \sqrt{2}(\mathbf{v}_3, \mathbf{v}_l),$$

or

$$k\big(13\sqrt{2} - 7\sqrt{6}\big) > \sqrt{6}(\mathbf{v}_2, \mathbf{v}_l) - \sqrt{2}(\mathbf{v}_3, \mathbf{v}_l).$$

Thus, for $l = 2$ the inequality is true for all $k > 0.53$; for $l = 3$ or 4 it is true for all $k \geqslant 0$. Notice that for $l = 2$ and $k = 0$, we get $b = 2$.

(ii) For $a = 4$, if $b = 4k + 2$ then the inequality is true for all $k > 1.72$. For this reason, the inequality between $R_2(4; 2, 6)$ and $R_2(4; 3, 6)$ is reversed. If $b = 4k + 3$ the inequality is true for all $k \geqslant 0$. □

Empirical evidence suggests that $R_2(a; 2, b) < R_2(a; 3, b)$ for all $a \geqslant 6$ and $b \geqslant 3$. We do not give a formal proof.

Lemma 9. *For all $a \geqslant 3$, $R_2(a; 2, a) < R_2(a; 3, a)$.*

Table 5
$A(a)$, $a \equiv 0, 1 \bmod 2$ and $B(a)$, $a \equiv 0, 1, 2 \bmod 3$

$a \bmod 2$	A
0	$\frac{\sqrt{2a}}{8}(3a-2)$
1	$\frac{1}{2\sqrt{\lfloor a/2 \rfloor}}(a+\lfloor a/2 \rfloor)(a-1-\lfloor a/2 \rfloor)$
$a \bmod 3$	B
0	$\frac{\sqrt{15a}}{90}(13a-9)$
1	$\frac{a(a-1)-3/2\lfloor a/3 \rfloor-5/2\lfloor a/3 \rfloor^2}{2\sqrt{a-1-7/2\lfloor a/3 \rfloor}}$
2	$\frac{a(a-1)-1-7/2\lfloor a/3 \rfloor-5/2\lfloor a/3 \rfloor^2}{\sqrt{4a+7-7\lfloor a/3 \rfloor}}$

Proof. If $a=3$ then $R_2(3;3,3) > R_2(3;2,3)$. For all $a \geqslant 4$, we have to show that $B(a) > A(a)$, where

$$A(a) = R_2(a;2,a)|\mathbf{v}_a| \quad \text{and} \quad B(a) = R_2(a;3,a)|\mathbf{v}_a|.$$

The formulas for $A(a)$, $a \equiv 0, 1 \bmod 2$ and $B(a)$, $a \equiv 0, 1, 2 \bmod 3$ are given in Table 5.

One can easily check in all six cases that $B(a) > A(a)$. □

Lemma 10. *For each $a \geqslant 3$ and each $b, c \geqslant 2$*

$$R_2(a;b,c) \geqslant \min\bigl(R_2(a;l',a), R_2(a;l,a), R_2(a;l',l)\bigr)$$

where $b \equiv l \bmod a$, $c \equiv l' \bmod a$.

Proof. If $l, l' \equiv 0, 1 \bmod a$, both $\mathbf{v}_b$ and $\mathbf{v}_c$ are on the ray R_a, and $R_2(a;b,c) = 1$.

If $l = l' = 2, \ldots, a-1$ then $\mathbf{v}_b$ and $\mathbf{v}_c$ belong to P_l and $R_2(a;b,c) \geqslant R_2(a;l,a)$.

Finally, if $l \neq l'$ one establishes the inequality by comparing the arcs on the unit sphere corresponding to the angles. These are the arcs between the points on the sphere on the rays generated by $\mathbf{v}_a$, $\mathbf{v}_l$, $\mathbf{v}_{l'}$, $\mathbf{v}_b$, and $\mathbf{v}_c$. □

To prove Conjecture 1 it suffices to show that

$$\min_{a \geqslant 3,\ b,c \geqslant 2} R_2(a;b,c) \geqslant R_2(5;2,3).$$

Let $R_2^*(a) = \min_{b,c \geqslant 2} R_2(a;b,c)$. According to Lemma 10, for each $a \geqslant 3$

$$R_2^*(a) = \min_{1<l,l'<a} \min\bigl(R_2(a;l',a), R_2(a;l,a), R_2(a;l',l)\bigr),$$

whence

$$\min_{a \geqslant 3,\ b,c \geqslant 2} R_2(a;b,c) = \min_{a \geqslant 3} R_2^*(a).$$

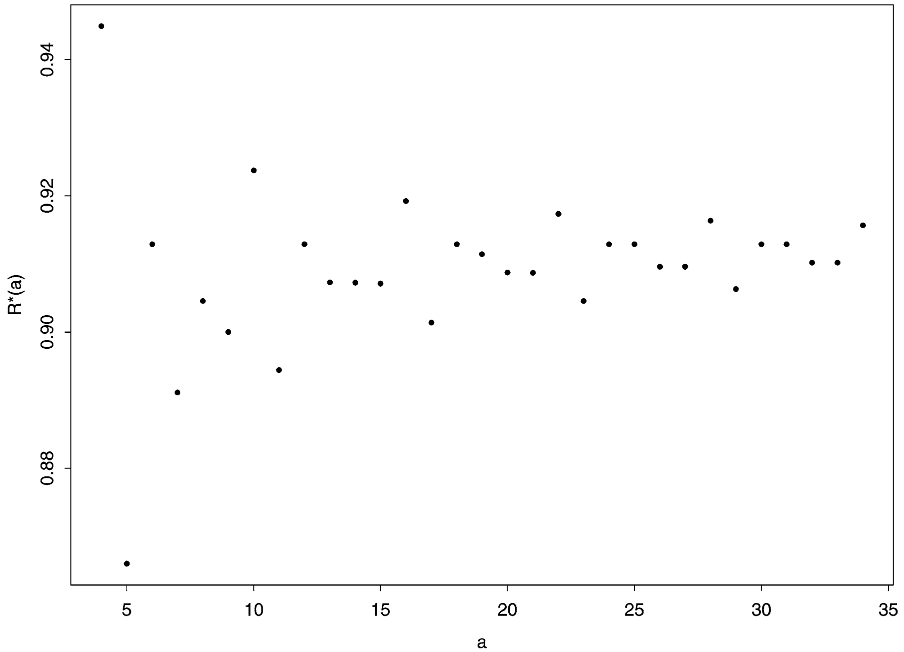

Fig. 4. $R_2^*(a)$ for $a = 3, \ldots, 35$.

In Fig. 4 we present a plot of $R_2^*(a)$ for $a = 3, \ldots, 35$. We see that in this range, $R_2(5; 2, 3)$ is the minimum, lending further credence to Conjecture 1.

6. Upper bounds for generalized Dedekind sums: Higher dimensions

6.1. Probability models

We introduce now a probability space and random variables, whose (mixed) moments yield the S- and M-functions. Let $\mathcal{D}_d^{(a)}$ be a d-dimensional discrete sample space, consisting of a^d points, that is,

$$\mathcal{D}_d^{(a)} = \left\{(m_1, \ldots, m_d)\colon\ m_j = 0, \ldots, a-1,\ j = 1, \ldots, d\right\}.$$

A point in $\mathcal{D}_d^{(a)}$ is a d-dimensional vector $\mathbf{m} = (m_1, \ldots, m_d)$. Consider the probability function on $\mathcal{D}_d^{(a)}$:

$$P(\mathbf{m}) = \begin{cases} 1/a, & \text{if } \mathbf{m} = j\mathbf{1}_d,\ j = 0, \ldots, a-1, \\ 0, & \text{otherwise}, \end{cases} \tag{6.1}$$

where $\mathbf{1}_d = (1, 1, 1, \dots, 1)$. This probability function is concentrated on the main diagonal points of $\mathcal{D}_d^{(a)}$. Define the random variables

$$X_i^{(a)}(\mathbf{m}; \mathbf{b}) = \begin{cases} \lfloor \frac{mb_i}{a} \rfloor, & \text{if } \mathbf{m} = m\mathbf{1}_d,\ m = 0, \dots, a-1, \\ 0, & \text{otherwise,} \end{cases} \tag{6.2}$$

where $\mathbf{b} = (b_1, \dots, b_d)$. It follows immediately that

$$S_d(a; \mathbf{b}) = E_P\left\{ \prod_{i=1}^{d} X_i^{(a)}(\mathbf{m}; \mathbf{b}) \right\}, \tag{6.3}$$

where $E_P\{\ \}$ denotes the expected value of the term in braces with respect to the probability function P. Moreover,

$$M_k(a; b_i) = E_P\left\{ \left(X_i^{(a)}(\mathbf{m}; \mathbf{b}) \right)^k \right\}. \tag{6.4}$$

Notice that $M_k(a; b_i)$ is the kth order moment of $X_i^{(a)}(\mathbf{m}; \mathbf{b})$. The Dilcher–Girstmair presentation of the S- and M-functions can be described as moments of the random variables

$$J_i^{(a)}(\mathbf{m}; \mathbf{b}) = \sum_{j=0}^{b_i - 1} j I\left\{ \mathbf{m}\colon \frac{ja}{b_i} \leqslant m_i < \frac{(j+1)a}{b_i} \right\}, \quad i = 1, \dots, d, \tag{6.5}$$

where $I\{\mathbf{m}\colon \dots\}$ is the indicator function. According to this definition,

$$S_d(a; \mathbf{b}) = E_P\left\{ \prod_{i=1}^{d} J_i^{(a)}(\mathbf{m}; \mathbf{b}) \right\} \tag{6.6}$$

and

$$M_k(a; b_i) = E_P\left\{ \left(J_i^{(a)}(\mathbf{m}; \mathbf{b}) \right)^k \right\}. \tag{6.7}$$

6.2. Upper bounds for $S_d(a; \mathbf{b})$

In the present section we use the random variables $X_i^{(a)}(\mathbf{m}; \mathbf{b})$. Since a and $\mathbf{b}$ are fixed, we will simplify the notation to calling the random variables $X_1, \dots, X_d$. Repeated application of the Cauchy–Schwartz inequality yields bounds in terms of the one-dimensional moments M. For example, for $d = 2$ we obtain

$$E\{X_1 X_2\} \leqslant \left(E\left\{X_1^2\right\} E\left\{X_2^2\right\} \right)^{1/2},$$

and thus

$$S_2(a; b_1, b_2) \leqslant \left(M_2(a, b_1) M_2(a, b_2) \right)^{1/2}.$$

For $d = 3$ we get

$$E\{X_1 X_2 X_3\} \leqslant \left(E\left\{X_1^2\right\} E\left\{X_2^2 X_3^2\right\}\right)^{1/2} \leqslant \left(E\left\{X_1^2\right\}\left(E\left\{X_2^4\right\} E\left\{X_3^4\right\}\right)^{1/2}\right)^{1/2}$$

or

$$S_3(a; b_1, b_2, b_3) \leqslant M_2^{1/2}(a, b_1) M_4^{1/4}(a, b_2) M_4^{1/4}(a, b_3). \tag{6.8}$$

By taking the geometric mean of the cyclical permutations, we get the symmetric upper bound

$$S_3(a; b_1, b_2, b_3) \leqslant \left(\prod_{j=1}^{3} M_2(a, b_j) M_4(a, b_j)\right)^{1/6}.$$

For $d = 4$ we similarly obtain

$$S_4(a; b_1, b_2, b_3, b_4) \leqslant \left(\prod_{j=1}^{4} M_4(a, b_j)\right)^{1/4}. \tag{6.9}$$

For $d = 5$ we start with

$$\begin{aligned} S_5(a; \mathbf{b}) &= E_P\{X_1 \cdots X_5\} \\ &\leqslant \left(E_P\left\{X_1^2 X_2^2\right\}\right)^{1/2} \left(E_P\left\{X_3^2 X_4^2 X_5^2\right\}\right)^{1/2} \\ &\leqslant \left(M_4(a; b_1) M_4(a; b_2)\right)^{1/4} \left(\prod_{j=3}^{5} M_4(a; b_j) M_8(a; b_j)\right)^{1/12}. \end{aligned}$$

Symmetrizing this upper bound by taking the geometric mean of the $\binom{5}{2}$ different bounds obtained by different selections of pairs and triplets gives

$$S_5(a; \mathbf{b}) \leqslant \left(\prod_{j=1}^{5} M_4^3(a; b_j) M_8(a; b_j)\right)^{1/20}. \tag{6.10}$$

From the upper bound for S_3 we immediately obtain

$$S_6(a; \mathbf{b}) \leqslant \left(\prod_{j=1}^{6} M_4(a; b_j) M_8(a; b_j)\right)^{1/12}. \tag{6.11}$$

Generally, if $d = 2k$, $k = 1, 2, \ldots,$ we have

$$S_{2k}(a; \mathbf{b}) \leqslant \left(E_P\left\{X_1^2 \cdots X_k^2\right\}\right)^{1/2} \left(E_P\left\{X_{k+1}^2 \cdots X_{2k}^2\right\}\right)^{1/2}, \tag{6.12}$$

from which we get, by utilizing previous results, symmetric upper bounds. For example,

$$\begin{aligned} S_8(a;\mathbf{b}) &\leqslant \bigl(M_8(a;b_1)\cdots M_8(a;b_4)\bigr)^{1/8}\bigl(M_8(a;b_5)\cdots M_8(a;b_8)\bigr)^{1/8} \\ &= \bigl(M_8(a;b_1)\cdots M_8(a;b_8)\bigr)^{1/8}, \end{aligned} \tag{6.13}$$

and

$$S_{10}(a;\mathbf{b}) \leqslant \left(\prod_{j=1}^{10} M_8^3(a;b_j)M_{16}(a;b_j)\right)^{1/40}. \tag{6.14}$$

We can immediately prove by induction the following:

Lemma 11.

$$S_{2^k}(a;\mathbf{b}) \leqslant \left(\prod_{j=1}^{2^k} M_{2^k}(a;b_j)\right)^{1/2^k}, \quad k=1,2,\ldots. \tag{6.15}$$

Similarly, for $k=0,1,\ldots$

$$S_{3\cdot 2^k}(a;\mathbf{b}) \leqslant \left(\prod_{j=1}^{3\cdot 2^k} M_{2^{k+1}}(a;b_j)M_{2^{k+2}}(a;b_j)\right)^{1/6\cdot 2^k} \tag{6.16}$$

and

$$S_{5\cdot 2^k}(a;\mathbf{b}) \leqslant \left(\prod_{j=1}^{5\cdot 2^k} M^3_{2^{k+2}}(a;b_j)M_{2^{k+3}}(a;b_j)\right)^{1/20\cdot 2^k}. \tag{6.17}$$

If $d=2k+1$ one needs a two-stage process of first partitioning to

$$\left(E_P\left\{\prod_{j=1}^{k} X_j^2\right\}\right)^{1/2}\left(E_P\left\{\prod_{j=1}^{k+1} X_{k+j}^2\right\}\right)^{1/2}$$

and then symmetrizing.

Before concluding this section, we remark that the above upper bounds for the S-functions are generally not unique. By different partitions one can obtain different bounds. For example, in the case of S_5, one could start with

$$E_P\{X_1\cdots X_5\} \leqslant \bigl(E_P\{X_1^2\}\bigr)^{1/2}\bigl(E_P\{X_2^2\cdots X_5^2\}\bigr)^{1/2} = \bigl(M_2(a;b_1)\bigr)^{1/2}\left(\prod_{j=2}^{5} M_8(a;b_j)\right)^{1/8}.$$

Table 6
Some values and bounds of S_5

a	$\mathbf{b}$	S_5	bound (6.10)	bound (6.18)	R_5
31	(3, 5, 7, 11, 13)	1213.806	1321.321	1456.985	0.9186
21	(5, 7, 9, 11, 13)	4411.333	4668.719	5190.201	0.9449
23	(5, 9, 11, 13, 17)	11429.74	12050.58	13385.72	0.9485
27	(5, 11, 13, 17, 21)	28101.93	29617.94	33011.8	0.9488
33	(7, 11, 13, 19, 23)	51943.76	54384.26	60525.59	0.9551

After symmetrization we get

$$S_5(a;\mathbf{b}) \leqslant \left(\prod_{j=1}^{5} M_2(a;b_j)M_8(a;b_j)\right)^{1/10}. \tag{6.18}$$

The question is which upper bound should be used, (6.10) or (6.18)? For example, if $a = 31$ and $\mathbf{b} = (3, 5, 7, 11, 13)$ then $S_5(a;\mathbf{b}) = 1213.806$. The upper bound given by (6.10) is 1321.321, whereas that given by (6.18) is 1456.985. In Table 6 we present some exact values of $S_5(a;\mathbf{b})$ and the two bounds (6.10) and (6.18). We also show $R_5(a;\mathbf{b})$, the ratio of $S_5(a;\mathbf{b})$ to the upper bound (6.10).

It seems from Table 6 that the upper bound given by (6.10) is closer to the exact value of $S_5(a;\mathbf{b})$ than (6.18). It is the preferred upper bound. It is also interesting that, like in the case of $R_2(a;\mathbf{b})$, all values of $R_5(a;\mathbf{b})$ in Table 6 are greater than 0.9186.

6.3. Relationships to upper bounds revisited

We study now upper bounds to S_d of the type given by (6.8)–(6.17). In particular, define

$$R_3(a;\mathbf{b}) = \frac{S_3(a;\mathbf{b})}{\left(\prod_{j=1}^{3} M_2(a,b_j)M_4(a,b_j)\right)^{1/6}}, \tag{6.19}$$

$$R_4(a;\mathbf{b}) = \frac{S_4(a;\mathbf{b})}{\left(\prod_{j=1}^{4} M_4(a,b_j)\right)^{1/4}}, \quad \text{and} \tag{6.20}$$

$$R_5(a;\mathbf{b}) = \frac{S_5(a;\mathbf{b})}{\left(\prod_{j=1}^{5} M_4^3(a;b_j)M_8(a;b_j)\right)^{1/20}}. \tag{6.21}$$

A few values of $R_5(a;\mathbf{b})$ are given in Table 6. It seems that the minimal $R_5(a;\mathbf{b})$ value is $R_5(7; 2, 3, 4, 5, 6) = 0.8567$. It is also interesting to observe that R_5, as shown in Table 6, is generally above 0.9, as in the case of R_2, despite the increase in dimension from 2 to 5. We try to explain this phenomenon in probability terms.

As shown in (6.3) and (6.6),

$$S_d(a;\mathbf{b}) = E_P\{X_1 \cdots X_d\} = E_P\{J_1 \cdots J_d\}.$$

Consider the case $d = 2$. According to the law of iterated expectation [1],

$$S_2(a; b_1, b_2) = E_P\left\{J^{(a)}(\mathbf{m}; b_1) E_P\left\{J^{(a)}(\mathbf{m}; b_2) \mid J^{(a)}(\mathbf{m}; b_1)\right\}\right\}, \tag{6.22}$$

where the second term on the right-hand side is the *conditional expectation* of $J^{(a)}(\mathbf{m}; b_2)$, given $J^{(a)}(\mathbf{m}; b_1)$. Notice that in the notation of Section 3,

$$S_2(a; b, c) = \frac{1}{a} \sum_{j=0}^{b-1} \sum_{l=0}^{c-1} jl f_{a;b,c}(j, l) = \frac{1}{a} \sum_{j=0}^{b-1} j f_{a;b}(j) \sum_{l=0}^{c-1} l \frac{f_{a;b,c}(j, l)}{f_{a;b}(j)}. \tag{6.23}$$

The key to understanding the phenomenon is that the joint frequencies $f_{a;b,c}(j, l)$ are distributed along the main diagonal, as illustrated in Table 1. In the special case that $b = c$,

$$f_{a;b,c}(j, l) = \begin{cases} f_{a;b}(j) = f_{a;c}(j), & \text{if } j \neq l, \\ 0, & \text{otherwise.} \end{cases}$$

In this case,

$$\sum_{l=0}^{b-1} l \frac{f_{a;b,c}(j, l)}{f_{a;b}(j)} = j \quad \text{and}$$

$$S_2(a; b, b) = \frac{1}{a} \sum_{j=0}^{b-1} j^2 f_{a;b}(j) = M_2(a; b),$$

as expected. When $b \neq c$ then R_2 is always smaller than 1, but might be quite close to it, even when b and c are different. For example, $R_2(50; 7, 13) = 0.9955$.

6.4. One-dimensional moments relationships

We present here some inequalities between $M_r(a; b)$ for fixed values of a and b and for variable r.

Theorem 12. *$M_r(a; b)$ is log-convex in r. That is,*

$$M_{2r}(a; b) M_{2r+2}(a; b) - M_{2r+1}^2(a; b) > 0. \tag{6.24}$$

Proof. First, by Liapounov's inequality of moments [6, p. 627] we have

$$M_1 < M_2^{1/2} < M_3^{1/3} < \cdots.$$

By factoring $\lfloor \ldots \rfloor^{2r+1} = \lfloor \ldots \rfloor^{r} \lfloor \ldots \rfloor^{r+1}$ we obtain the inequality

$$M_{2r+1}^2(a; b) < M_{2r}(a; b) M_{2r+2}(a; b) \tag{6.25}$$

for all $r \geqslant 1$. That is, $M_r(a; b)$ is log-convex in r. $\square$

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Appendix

Algorithm for determining $f_b^a(i)$, $i = 0, \dots, b-1$

```
STEP 0. Set:
       (i)    r = a/b;
      (ii)    l = a-b*[r];
     (iii)    f = O(1,b);  # b-dimensional vector of zeros

STEP 1. Compute:
    f[0] <- 1+[r];
    f[i] <- [(i+1)*r]-[i*r], i=1,...,(b-2);
    f[b-1] <- a-1-[(b-1)*r];

STEP 2.
    IF ((l=0) or (b=2)) {GOTO STEP 3};
    ELSE {
        FOR (i=1,...,b-2) {
            IF ([(i+1)*r] = r*(i+1)) {
                f[i] <- f[i]-1;
                f[i+1] <- f[i+1]+1;
            }
        }
    }

STEP 3. PRINT f

END.
```

Algorithm for determining $f_{bc}^a(i, j)$

```
STEP 0. Set:
    r1 <- a/b;
    r2 <- a/c;
    l1 <- a-b*[r1];
    l2 <- a-c*[r2];
    CT <- O((b+1),(c+1));  # matrix of zeros,
                           # of dimensions (b+1)*(c+1)
    t1 <- O(b,1);
    t2 <- O(1,c);
```

```
STEP 1. Compute:
    CT[i,(c+1)] <- f_b[i-1], i=1,...,b;
    CT[(b+1), j] <- f_c[j-1], j=1,...,c;
    CT[(b+1),(c+1)] <- a;
    CT[1,1] <- min(CT[1,c+1], CT[b+1,1]);
    t2[1] <- t2[1] + CT[1,1];

STEP 2. Compute:
    FOR (i=2,...,b) {
    CT[i,1] <- max(0, min(f_c[1]-t2[1], f_b[i-1]));
    t2[1] <- t2[1] + CT[i,1];
    }
    t1 <- CT[1:b,1];

STEP 3. Compute:
    FOR (j=2,...,c) {
    CT[1,j] <- max(0, min(f_b[0]-t1[1], f_c[j-1]));
    t1[1] <- t1[1] + CT[1,j];
    t2[j] <- t2[j] + CT[1,j];
    }

STEP 4. Compute:
    FOR (i=2,...,b) {
        FOR (j=2,...,c) {
        cty <- max(0, min(f_b[i-1]- t1[i], f_c[j-1]));
        ctx <- max(0, min(f_c[j-1]-t2[j], f_b[i-1]));
        CT[i,j] <- min(ctx,cty);
        t1[i] <- t1[i]+  CT[i,j];
        t2[j] <- t2[j] + CT[i,j];
        }
    }

STEP 5. PRINT CT

END.
```

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